Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Possible superconductivity in hetero-polar interfaces of CuCl/Si superlattices: (001) and (111)[1] S. H. RHIM, R. SANIZ, A.J. FREEMAN, Northwestern U,, J.J. YU, Seoul Natl. U. — To investigate possible interfacial superconductivity[2] in CuCl/Si superlattices, we carried out first-principles calculations using the highly precise FLAPW [3] method. Two possible growth directions, (001) and (111), are compared through their band structures, density of states (DOS), charge densities and Fermi surfaces. While the (111) superlattice is always metallic, the (001) superlattice is metallic or insulating depending on the number of Si and CuCl layers. Both directions exhibit two dimensional (2D) character at the interfaces which is a result of charge transfer between CuCl and Si layers. For metallic superlattices, the 2D conduction bands at the interfaces, resemble the 2D Cu-O $dp\sigma$ bands of cuprate superconductors. To obtain T_C based on conventional electron-phonon (e-p) interactions, we calculated the e-p coupling constant, λ, within the rigid muffin-tin approximation.[4] The results indicate that while e-p coupling is present in both directions, it gives $T_C = 0.41 \sim 1.69$ K, i.e. one order of magnitude lower than the previously reported high transition temperature[2]- which, if confirmed, would indicate a possible role for excitonic effects.

[1]DOE (DE-F602-88ER45372/A022))
[2]%Mattes, %Physica C **162**,554 (1989); Mattes and Foiles, Physica 135B, 139 (1985)
[3]Wimmer, Krakauer, Weinert, and Freeman, Phys.Rev.B, **24**, 864 (1981)
[4]Gaspari and Gyoffry, Phys. Rev. Lett. **28**, 801, (1972)

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Date submitted: 07 Dec 2005 Electronic form version 1.4